Semiconductor Process Modeling

Computer simulation of particle beam/laser effects in next-generation integrated circuit manufacturing

We are using LLNL-developed computer codes to model energetic particle interactions with solids and surfaces in next-generation integrated circuit production processes. These codes, called molecular dynamics (MD) tools, use state-of-the-art massively parallel computers to provide an atom-level view of the diffusion process and defects produced during ion-beam-assisted processing of materials.

Process improvement applications

These simulation codes are leading the way toward development of a process-modeling package for next-generation semiconductor integrated circuit component manufacturing.

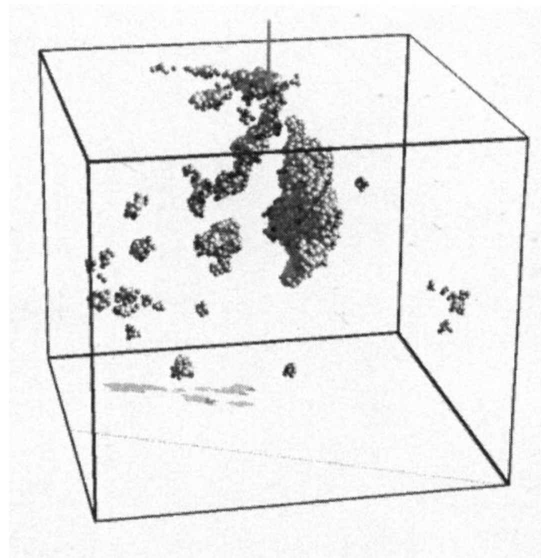
Rapid thermal annealing—Our MD simulations are providing us with a complete description of the state of the silicon lattice following high-dose, low-energy implantation of dopants. These simulations will soon allow us to predict how a dopant diffuses during rapid thermal annealing for a given set of implantation conditions.

Cluster beam implantation—Cluster beams (ionized and accelerated clusters of particles) offer unique new opportunities for the manufacturing of semiconductor components. However, their interaction with a solid surface results in a microstructure different from that produced by individual ion implantation. MD simulation offers a unique tool to study the conditions required to produce damage-free shallow junctions in silicon.

Gas immersion laser doping—Excimer laser-based gas immersion doping of semiconductors is a promising novel technique for the manufacturing of abrupt shallow junctions. Critical to the development of this method is understanding the behavior of silicon and dopants when they are exposed to the laser. Our MD simulation tools are ideal to study the kinetics of diffusion in the rapidly moving recrystallization front, formed when silicon is turned into liquid and back into solid. Our studies will lead the way toward more abrupt shallow junctions.

APPLICATIONS

- *Ultra-shallow junction technology development*
- *Recrystallization of solid/liquid silicon interfaces for flat-panel display technology*
- *Transient enhanced diffusion of dopants during rapid thermal annealing*



Computer simulation illustrates defects and amorphous zones in silicon after implantation with 10-keV silicon ions.

Requirements: To use these codes, massively parallel computing capability is necessary. Industrial partners are invited to utilize the capability at LLNL.

Availability: These codes are available now. LLNL is seeking industrial partners to develop and commercialize this technology computer-aided design package to apply it to next generation semiconductor process modeling.

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